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**FINAL REPORT**

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**Title: Correlation of Burning Rates and Energy Transport  
Mechanisms in Open and Enclosed Liquid Pool Fires**

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## I. OBJECTIVE

A full scale fire model for an enclosed environment needs a quantitative description of the fire source itself. This is because of the time dependent power output of a flame arising from oxygen depletion.

The objective of this research was to develop a quantitative understanding of the behavior of simulated gas flames and liquid pool fires of low initial momentum (buoyancy controlled) in a two-dimensional, axi-symmetric situation. Specifically, we predicted velocity, temperature and species concentration fields as a function of axial and radial coordinates. Knowing these fields, we can estimate the quantity of feed back energy which in turn determines the mass burning rate of a liquid pool. This enables us to determine the power output of the fire source in question, as a function of the chamber environment.

Statement "A" per telecon Dr. F. Williams  
Naval Research Laboratory/code 6183.

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## II. MODEL FORMULATION

A brief description of our model is presented here. The model to be described has been developed over the last 3 years. Those features incorporated during this past year are indicated in Section III below.

### 1. Mathematical

The conservation expressions for all of the variables are written in the parabolic form, for an axi-symmetric flame :

Mass :

$$\frac{\partial(\rho\bar{U})}{\partial z} + \frac{1}{y} \frac{\partial(y\rho\bar{V})}{\partial y} = 0. \quad (1)$$

Momentum and all scalar quantities :

$$\bar{\rho}\bar{U} \frac{\partial\Phi}{\partial z} + \bar{\rho}\bar{V} \frac{\partial\Phi}{\partial y} = \frac{1}{y} \frac{\partial}{\partial y} \left( y \mu_t \frac{\partial\Phi}{\partial y} \right) + R\phi. \quad (2)$$

The variables  $\Phi$ , the Prandtl/Schmidt numbers  $\sigma\phi$ , and the source terms  $R\phi$  have been tabulated previously. The effective turbulent viscosity is given by

$$\mu_t = \rho C_D \kappa^2 / \varepsilon. \quad (3)$$

The boundary conditions irrespective of the initial conditions employed are :

$$\frac{\partial\Phi}{\partial y} = 0 \text{ at } y=0 \text{ and } \Phi=0 \text{ at } y=\infty.$$

The differential equations for fuel mass fraction ( $m_{fu}$ ) and the conserved scalar (mixture fraction),  $f$ , are solved within this framework. The mass fractions of the species  $O_2$  ( $m_{O_2}$ ),  $CO_2$  ( $m_{CO_2}$ ),  $H_2O$  ( $m_{H_2O}$ ) and  $N_2$  ( $m_{N_2}$ ) are obtained from

the auxiliary relations:

$$f = (\varphi - \varphi_0) / (\varphi_F - \varphi_0) ; \quad (4.a)$$

$$\varphi = m_{fu} - m_{O_2} / r_{fu} \quad (4.b)$$

$$= m_{fu} + m_{CO_2} / i_{CO_2} \quad (4.c)$$

$$= m_{fu} + m_{H_2O} / i_{H_2O} \quad (4.d)$$

$$= m_{N_2} ; \quad (4.c)$$

$$\sum_{\text{all } j} m_j = 1. \quad (4.d)$$

Here, the subscripts F and O refer to the fuel bearing and oxygen bearing streams respectively; and the i's are the masses of the species  $CO_2$  and  $H_2O$  produced by the reaction of a unit mass of fuel.

The specific enthalpy,  $h$ , is defined by

$$h = C_p T + (1-X_R)\Delta H m_{fu} \quad (5)$$

where  $C_p$  is the specific heat,  $\Delta H$  is the heat of combustion, and  $X_R$  is the radiative fraction.

The temperature dependence of the laminar viscosity,  $\mu$ , is given by the relation,

$$\mu = \mu_0 (T / T_a)^{0.5} \sum m_j, \quad (6)$$

where  $\mu_0$  is the viscosity at a reference temperature,  $T_a$ .

The main flow field is assumed to be parabolic. This assumption may be invalid close to the burner exit, hence some error may exist in the near field predictions. However, similar parabolic flow field approximations have been made by other authors. The usual two equation model is employed to describe the turbulence, which can be

characterized by the turbulent kinetic energy,  $\kappa$ , and the kinetic energy dissipation rate,  $\epsilon$ .

## 2. The Combustion Model

The chemical kinetics are assumed to be infinitely fast. However, the microscale processes responsible for the turbulence dissipation and molecular mixing in the turbulent field are typically intermittent and certainly not infinitely fast.

Magnussen has proposed a physical and conceptual model for the interaction of the turbulence and chemistry for both premixed and diffusion flames. In this model the chemical reactions take place in various reactive zones or fine structures. The reaction rate is then expressed in terms of the mass transfer into the fine structures from the surrounding fluid. Thus the overall reaction rate can given by the expression,

$$R_{fu} = \frac{\dot{m} x}{(1-x)^{r_{fu}}} C_{min}, \quad (7)$$

where  $C_{min}$  is the smaller of  $C_{fu}$  and  $C_{O_2}/r_{fu}$ , which indicate the concentration of fuel and oxygen in the fluid respectively. Here  $r_{fu}$  is the stoichiometric oxygen requirement.  $x$  is a factor between zero and one which was introduced by Magnussen for premixed flames to require the presence of products in a region before reaction could occur. Since we are working with diffusion flames where this is inappropriate, we set  $x$  equal to one.

The quantity  $m$  is the mass transfer rate between the fine structures and the bulk of the fluid; they can be defined in terms of  $\kappa$  and  $\epsilon$  and the kinematic isotropic viscosity  $\nu$  as follows;

$$m = 23.6 \left( \frac{\nu \epsilon}{\kappa^2} \right)^{1/4} \frac{\epsilon}{\kappa} . \quad (8)$$

$\tau^*$  is the fraction of the fluid contained within the fine structures as given by

$$\tau^* = 9.7 \left( \frac{\nu \epsilon}{\kappa^2} \right)^{3/4} . \quad (9)$$

The chemical source term in the fuel conservation expression is thus given by Eq.(7). This chemistry-turbulence source is attractive both in terms of its applicability to fire problems, and to both premixed and diffusion flame situations.

### 3. Radiation

The lack of understanding and development of radiative heat transfer models in fires is primarily due to the lack of accurate flame property data needed as primary input parameters.

Considering the self absorbing and emitting non-homogeneous media in fires, as well as in the present pool-like gas flames, we chose to use a flux model for radiation modeling. Although this model has been utilized for applied combustion problems such as in cylindrical furnaces, the applicability to fires where a strong buoyant field exists seems to be untested as yet. In previous work, we used the

four flux model and employed the gray gas approximation on gaseous as well as liquid pool fires of moderate size using absorption coefficients as input parameters. In the present work they are computed as described below, using the temperature weighted sum-gray gases model.

The radiative flux sum  $F$  in the radial and axial directions is given in the four-flux model as :

$$y^{-1} \frac{d}{dy} [y\Gamma_y \frac{dF_y}{dy}] = K(F_y - E) \quad (10)$$

and

$$\frac{d}{dz} [\Gamma_z \frac{dF_z}{dz}] = K(F_z - E) \quad (11)$$

where

$$\Gamma_y = y/(1+Ky) \text{ and } \Gamma_z = 1/K .$$

Here,  $K$  is the flux absorption coefficient ( $m^{-1}$ ).

The flux absorption coefficient  $K$  can be derived from the prevailing concentration and temperature fields in the flame, and the optical path length as described below. The total emissivity in the weighted sum-gray gases model is evaluated from the expression

$$\varepsilon_m = \sum_{i=0}^I a_{em,i}(T) [1 - \exp(-k_i P S)] \quad (12)$$

where the  $a_{em,i}$  represent the emissivity weighting factors for the  $i^{\text{th}}$  gray gas based on the gas temperature,  $T$ .  $k_i$  is the absorption coefficient,  $P$  is the partial pressure of the absorbing gases, and  $S$  is the path length. The weight factor  $a_{em,i}$  is physically interpreted as the fractional

amount of black body energy in the spectral region where the gray gas absorption coefficient,  $\kappa_i$ , exists.

A relation between the true absorption coefficient,  $k$ , and the flux absorption coefficient,  $K$ , can be established by assuming thermal equilibrium, which implies that the local cell absorptivity and the emissivity are equal. Then the absorption coefficient  $k$  is determined by

$$k = \epsilon_m / \delta n , \quad (13)$$

where  $\delta n$  is the cell dimension. The flux absorption coefficient  $K$  is equal to  $\kappa_i$  or  $2k$  depending on the distribution of the radiation intensity. In the present work,  $K = 2k$  was used implying an isotropic radiation intensity.

#### 4. Soot formation and radiation

In the absence of a detailed soot formation model for turbulent, diffusion flames, we have employed the phenomenological scheme of soot formation proposed by Tesner et al, which was later applied to jet flames by Magnusson. The soot formation process depends on the formation of some active radical particles. From these particles, soot particles grow. The formation rate of radical nuclei is given by:

$$R_{n,f} = n_0 + (f-g)n - g_0 n N \quad (\text{part/m}^3/\text{s}) \quad (14)$$

where  $n$  is the concentration of radical nuclei,  $N$  is the concentration of soot particles, and  $n_0$  is the rate of spontaneous formation of radical nuclei,

$$n_0 = a_0 C_{fu} \exp(-E/RT) \quad (\text{part/m}^3/\text{s}). \quad (15)$$

Above,  $C_{fu}$  is the mean concentration of fuel ( $\text{kg/m}^3$ ), and  $f$ ,  $g$ , and  $g_0$  are certain constants. The rate of soot formation is expressed by

$$R_{s,f} = m_p (a - bN) n \quad (\text{Kg/m}^3/\text{s}), \quad (16)$$

where  $m_p$  is the mass of the soot particle ( $\text{Kg/part}$ ), and  $a$  and  $b$  are constants.

The soot and radical nuclei are formed and burnt in the flame zone. The mean rate of nucleus and soot particle combustion are expressed as follows :

$$R_{n,c} = R_{fu} n / C_{fu} \quad (\text{part/m}^3/\text{s}) \quad (17)$$

and

$$R_{s,c} = R_{fu} C_s / C_{fu} \quad (\text{kg/m}^3/\text{s}), \quad (18)$$

where  $C_s$  is the soot concentration ( $\text{Kg/m}^3$ ).

The absorption coefficients referred to earlier are updated for the calculation of the overall absorption coefficients of the soot + gas mixture by the relation

$$k = k_g + K_s - K_g K_s, \quad (19)$$

where  $k_g$  is the absorption coefficient due to the gas only and  $k_s$  is the absorption coefficient of the soot. The soot absorption is approximately expressed by:

$$k_s = 4.38 \cdot 10^{-4} C_s T \quad (20)$$

## 5. Solution procedure

The mathematical model described in the previous section is given by a set of partial differential equations which are all parabolic except for the axial radiation. All of these parabolic expressions are solved by the marching

9

technique using a modified GENMIX code. However, the axial flux sum,  $F_z$ , is elliptic and not compatible with the same process and therefore needs special attention. The axial flux sum  $F_z$  is solved separately using the Tri-Diagonal-Matrix Algorithm (TDMA) and the temperature field was updated. The GENMIX code employs a floating grid in the radial direction. We employ 50 grid nodes over the half width of the flame. A maximum axial step size corresponding to 0.1% of the current width of the flame is employed.

## V. ACCOMPLISHMENTS ( Nov. 15, 1986 - February 28, 1988)

During this contract period we completed the following tasks:

### 1. Application to liquid pool fires

Figure 1 summarizes the predicted visible flame height as a function of the reduced calorific output coordinate  $Q^*$  for various liquid pool fires (methanol, heptane, kerosene, and gasoline). Results for gas flames of propane and methane are also included here. The quantity  $Q^*$  is defined as

$$Q^* = [ Q / \rho C_p T_s g^{1/2} ]^{2/5} \quad (21)$$

where  $Q$  is the calorific output of the flame,  $\rho$  is the density of the fuel vapor,  $T_s$  is the fuel surface temperature, and  $g$  is the acceleration due to gravity. The visible flame height,  $Z_v$ , is obtained from the centerline temperature profile. The ratio  $Z_v/Q^*$  is about 4.5 and is consistent with the value for buoyant flames. The predicted

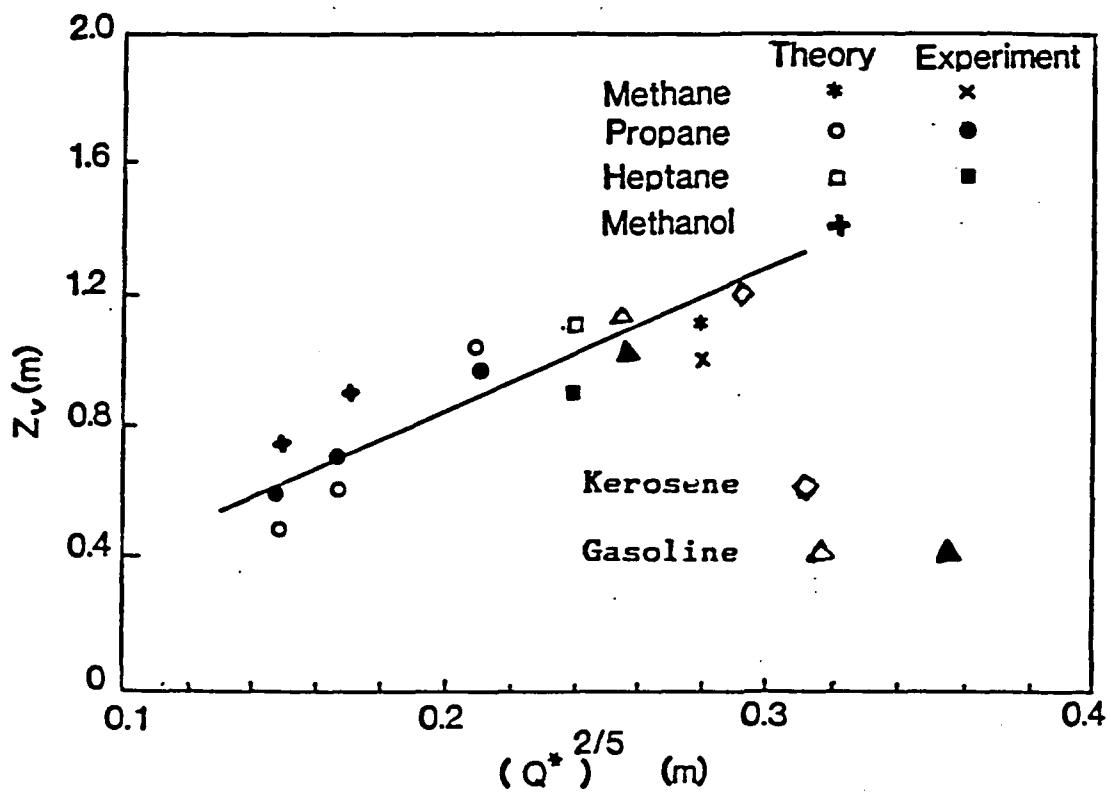


figure 1: Comparison of Visible Flame Height ( $Z_v$ ) Predicted and Reported.  $Q^*$  is reduced coordinate.

flame heights are in reasonable agreement with experiment.

We need to point out here that we did not calculate the mass burning rate for these liquid pool fires, but rather assumed values obtained from experimental data.

2. Determination of initial boundary conditions for the turbulent quantities and application to propane flames.

During the course of our work, it was realized that optimization of the initial conditions for the  $\kappa$ -  $\epsilon$  turbulence quantities is needed for better reproduction of the flame behavior. Seemingly, the choice of initial conditions for  $\kappa$  and  $\epsilon$  are critical to the combustion model. Unfortunately, in the absence of measured inlet quantities, no simple or straightforward method seems to be available to handle this problem. As a practical solution to this problem, in our calculations the turbulent quantities were introduced at the burner exit by employing the following relations,

$$\kappa_0 = \alpha_k \cdot U_0^2, \quad (22)$$

$$\epsilon_0 = \alpha_e \cdot \kappa^{3/2} / r_1, \quad (23)$$

where  $\alpha_k$  and  $\alpha_e$  are variable parameters, and  $r_1$  is the radius of the burner exit. A systematic analysis was carried out to determine those values for  $\alpha_k$  and  $\alpha_e$  which gave the best overall flame behavior. Values of  $\alpha_k$  in the range  $10^{-4}$  to  $10^2$  and  $\alpha_e$  in the range  $10^{-1}$  to 10 were tested. The final values chosen in this study are those which give the best agreement with experiment for one of the

propane flames ( $\alpha_k = 10$ ,  $\alpha_e = 1$ ). The same constants were used in all the calculations for the other flames.

Figure 2A shows the variation of the mean temperature along the burner axis for a propane flame of 37.9 kW, with and without radiation. Accompanying experimental results are shown from Gengembre et al. The temperature field predicted without radiation is close to the experimental results except in the peak combustion zone where it is overestimated. Also, the downstream temperatures are slightly underestimated. Upon including radiation, the peak temperature as well as the downstream temperatures are in better agreement with experiment. The agreement in the temperature throughout means that the combustion zone height,  $Z_c$ , and the visible flame height,  $Z_v$ , defined as above, are well reproduced. The Wallburn model of Tamanini, clearly overestimates the temperature field below 100 cm. For the results in Fig. 2, only gaseous radiation is considered and radiation by soot particles is not explicitly included in the model. A radiative fraction  $\alpha X_R$ , is considered to account for the total heat loss from the flame. Incorporation of soot radiation is considered in our further work on methane flames, to be described below. Figure 2B shows the centerline axial velocity of the same flame, with and without radiation. The agreement between our predicted and experimental results is generally good.

### 3. Inclusion of soot radiation and application to methane flames.

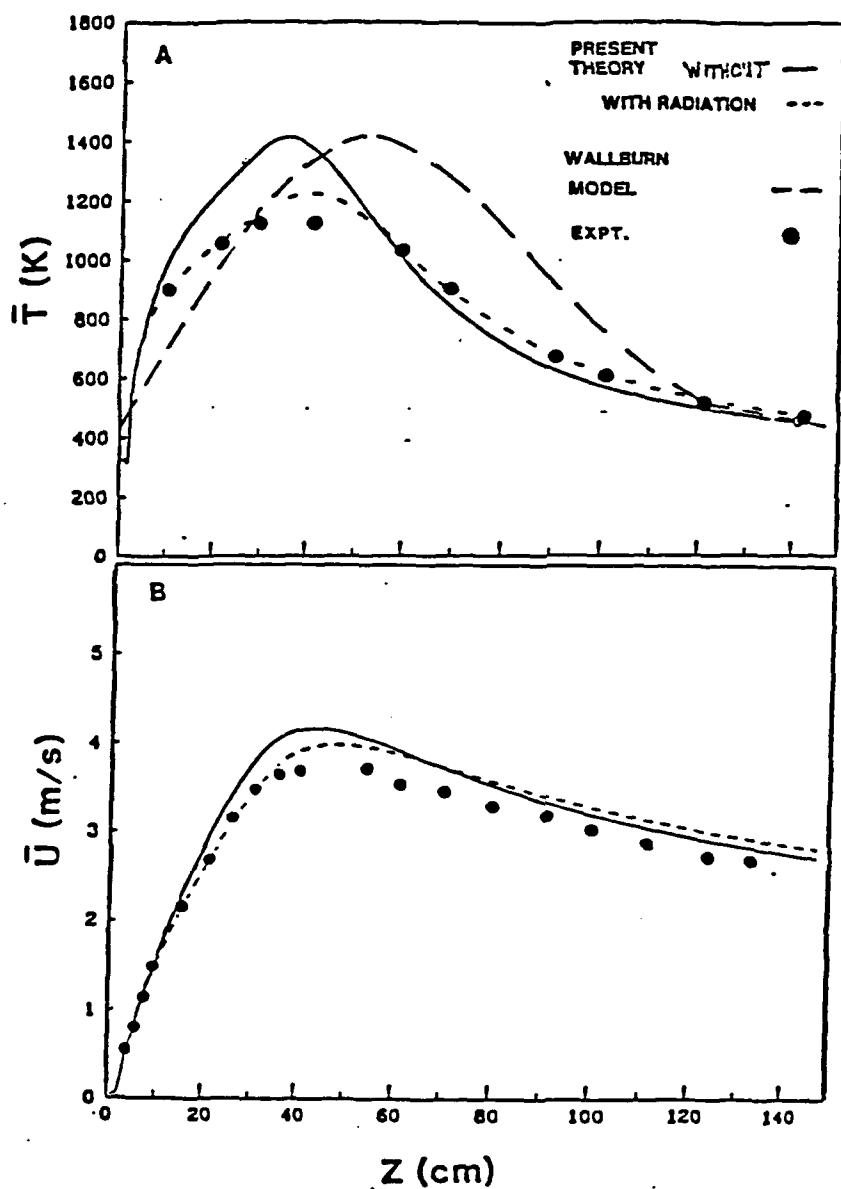


Figure 2 A: Comparison of predicted centerline mean temperature with the experiment for propane flame of 37.9 kW. Only gas radiation included. 2B: Comparison of predicted axial velocity along the centerline with the experiment

Figure 3A shows the temperature field of a methane flame along the centerline, predicted with and without radiation. Here soot formation was considered explicitly by solving the differential equations for soot and radical nuclei, as described above. The absorption coefficients of the soot + gas mixture was calculated using Eq.(19). The predicted temperature field is seen to be close to the experimental values as reported by Crawford et al. The soot concentration field is shown in Figure 3B. As seen, soot is formed in the fuel rich region and at the same time burnt. However, in the present case, soot is exhausted at the plume region, indicating a smoking tendency.

#### IV. SUMMARY

Our accomplishments during this past contract period can be summarized as follows:

1. Application of the field model to liquid pool fires of moderate size and comparison with experimental data. The agreement is generally good.
2. Optimization of the  $k-\epsilon$  initial conditions for burners of moderate size, and model validation using three propane flames of varying calorific power output. The radiation model was further augmented with a temperature weighted gray gas model.
3. Development of a model for soot formation and soot radiation and application of the model to methane flames with good agreement with experimental data.

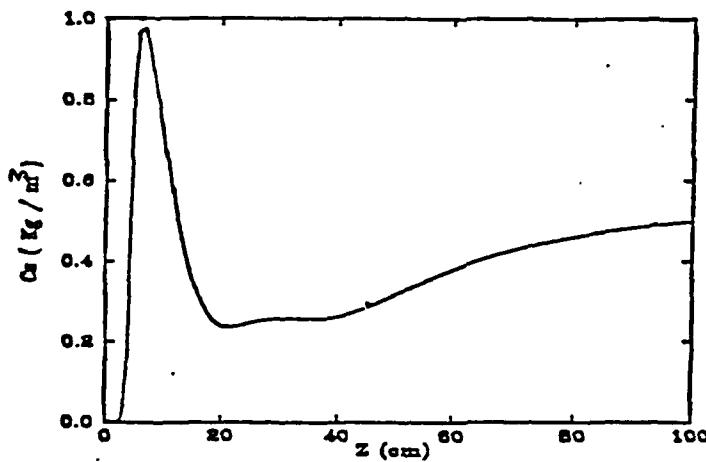
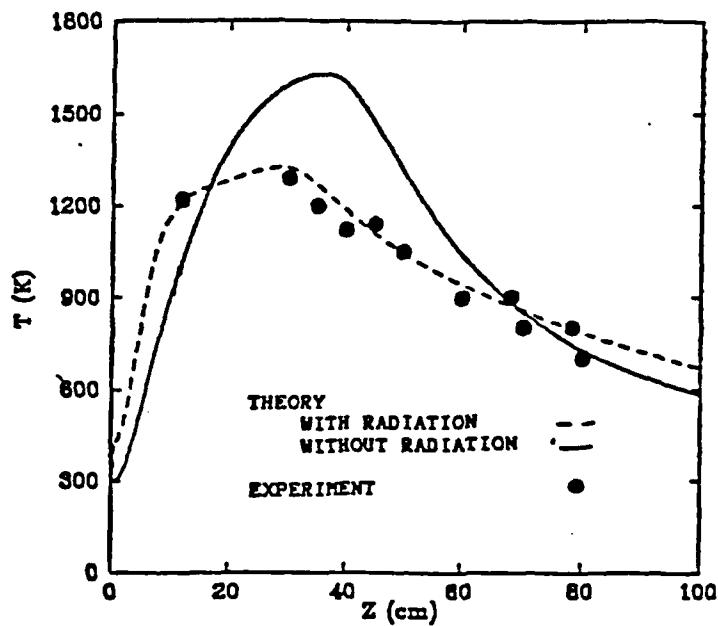


Figure 3A: Comparison of centerline mean temperature for methane flame of 28 kW. Soot radiation included in the model. 3B: Concentration of soot ( $C_s$ ) along the centerline for methane flame.

These accomplishments have been communicated in  
the following talks and papers :

1. " Numerical Modeling of Freely Burning Pool Fires ",  
paper presented at the International Meeting of Fire  
Research and Test Center, Avila, Spain, October, 1986.  
Vol. 1, p. 83 of Symposium Publication.
2. " Radiative Heat Transfer in Pool-Like Gas Flames ", a  
talk presented at the Fall Technical Meeting of The  
Eastern States Section of the Combustion Institute, San  
Juan, Puerto Rico, December, 1986
3. " Modeling Turbulent, Buoyant Pool-Like Gas Flames  
Including Radiative Heat Transfer " accepted for  
publication in Fire Safety Science.
4. " Numerical Simulation of Pool-Like Gas Flames of  
Methane With Special Emphasis on Soot Formation and  
Radiation ", Paper to be submitted to Fire Safety  
Science.